Fluctuation-dissipation relation for the Ising-Glauber model with arbitrary exchange couplings

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Abstract. We derive an exact expression of the response function to an infinitesimal magnetic field for the Ising-Glauber model with arbitrary exchange couplings. The result is expressed in terms of thermodynamic averages and does not depend on initial conditions or dimension of space. The comparison with the equilibrium case gives some understanding on the way the fluctuation-dissipation theorem is violated out-of-equilibrium.

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1. Introduction

The knowledge about out-of-equilibrium processes is far from being as advanced as for systems at equilibrium. In particular, the fluctuation-dissipation theorem (FDT) which holds at equilibrium is known to be violated out-of-equilibrium. This theorem states that at equilibrium the response function $R_{\rm eq}(t,s)$ at time t to an infinitesimal field branched to the system at time s is related to the time-derivative of the two-time autocorrelation function $C_{\rm eq}(t,s)$:

$$R_{\rm eq}(t,s) = \beta \frac{\partial C_{\rm eq}(t,s)}{\partial s}. \tag{1}$$

In the Ising case, the response function reads $R(t,s) = \frac{\delta \langle \sigma_i(t) \rangle}{\delta h_i(s)}$ and the correlation function $C(t,s) = \langle \sigma_i(t)\sigma_i(s)\rangle$. Based on a mean-field study of spin-glasses, Cugliandolo *et al* [1, 2] have conjectured that for asymptotically large times the FDT has to be corrected by a multiplicative factor $X(t,s)$ which moreover depends on time only through the correlation function:

$$R(t,s) = \beta X(C(t,s)) \frac{\partial C(t,s)}{\partial s}. \tag{2}$$

Exact results have been obtained for the ferromagnetic Ising chain [3, 4] that confirm this conjecture. The violation ratio $X(t,s)$ has been also numerically computed for many systems: 2d and 3d-Ising ferromagnets [5], 3d Edwards-Anderson model [6], 3d and 4d Gaussian Ising spin glasses [7], 2d Ising ferromagnet with dipolar interactions [8], ... The response function has been exactly calculated in the case of the Ising chain [9] but the result is not written in terms of thermodynamic averages making difficult any conjecture on the way the FDT is violated.

We present an analytic study of the Glauber dynamics of the Ising model with arbitrary exchange couplings. The response function to an infinitesimal magnetic field is first calculated at equilibrium and the compatibility with the fluctuation-dissipation theorem is verified. In the last section, the response function is derived out-of-equilibrium and the expression is compared to the equilibrium equivalent.

2. Model, dynamics and general response function

2.1. The model and its dynamics

We consider a classical Ising model whose degrees of freedom are scalar variables $\sigma_i = \pm 1$ located on the nodes of a d-dimensional lattice. Let us denote $\wp(\{\sigma\},t)$ the probability to observe the system in the state $\{\sigma\}$ at time t. The dynamics of the system is supposed to be governed by the master equation:

$$\frac{\partial \wp(\{\sigma\},t)}{\partial t} = \sum_{\{\sigma'\}} \Big[\wp(\{\sigma'\},t) W(\{\sigma'\} \to \{\sigma\}) - \wp(\{\sigma\},t) W(\{\sigma\} \to \{\sigma'\}) \Big] \tag{3}$$

where $W(\{\sigma\}\rightarrow\{\sigma'\})$ is the transition rate from the state $\{\sigma\}$ to the state $\{\sigma'\}$ per unit of time. The normation is written $\sum_{\{\sigma'\}}W(\{\sigma\}\rightarrow\{\sigma'\})=1$. The transition rates are defined by the stationarity condition

$$\sum_{\{\sigma'\}}\Big[\wp_{\rm eq}(\{\sigma'\})W(\{\sigma'\}\rightarrow\{\sigma\})-\wp_{\rm eq}(\{\sigma\})W(\{\sigma\}\rightarrow\{\sigma'\})\Big]=0 \qquad (4)$$

where $\wp_{\rm eq}(\{\sigma\})$ is the equilibrium probability distribution which reads for the Ising model with general exchange-couplings:

$$\wp_{\rm eq}(\{\sigma\})=\frac{1}{\mathcal{Z}}e^{-\beta\mathcal{H}(\{\sigma\})}=\frac{1}{\mathcal{Z}}e^{-\beta\sum_{k,l<k}J_{kl}\sigma_k\sigma_l}. \qquad (5)$$

Equation (4) is satisfied when the detailed balance holds:

$$\wp_{\rm eq}(\{\sigma'\})W(\{\sigma'\}\rightarrow\{\sigma\})=\wp_{\rm eq}(\{\sigma\})W(\{\sigma\}\rightarrow\{\sigma'\}). \qquad (6)$$

This last unnecessary but sufficient condition is fulfilled by the heat-bath single-spin flip dynamics defined by the following transition rates:

$$\begin{aligned}W(\{\sigma\}\rightarrow\{\sigma'\})&=\Big[\prod_{l\neq k}\delta_{\sigma_l,\sigma'_l}\Big]\frac{\sum_\sigma\delta_{\sigma'_k,\sigma}\wp_{\rm eq}(\{\sigma_l\}_{l\neq k},\sigma_k=\sigma)}{\sum_\sigma\wp_{\rm eq}(\{\sigma_l\}_{l\neq k},\sigma_k=\sigma)}\\&=\Big[\prod_{l\neq k}\delta_{\sigma_l,\sigma'_l}\Big]\frac{e^{-\beta\sum_{l\neq k}J_{kl}\sigma'_l\sigma'_k}}{\sum_{\sigma=\pm1}e^{-\beta\sum_{l\neq k}J_{kl}\sigma'_l\sigma}}. \qquad (7)\end{aligned}$$

Only the single-spin flip $\sigma_k\rightarrow\sigma'_k$ is allowed. The product of Kronecker deltas ensures that all other spins are not modified during the transition. The spin σ_k takes after the transition the new value σ'_k chosen according to the equilibrium probability distribution $\wp_{\rm eq}(\{\sigma\})$. All spins are successively updated during the evolution of the system. These transition rates reduce to Glauber's ones [9] in the case of the Ising chain.

2.2. The response function

A magnetic field h_i is coupled to the spin σ_i between the times s and $s+\Delta s$ where Δs is supposed to be small. Between these instants, the transition rates are changed to $W_h(\{\sigma\}\rightarrow\{\sigma'\})$ satisfying equation (7) with an additional term $\beta h_i\sigma_i$ in the Hamiltonian of the equilibrium probability distribution (5):

$$W_h(\{\sigma\}\rightarrow\{\sigma'\})=\Big[\prod_{l\neq k}\delta_{\sigma_l,\sigma'_l}\Big]\frac{e^{-\beta\left[\sum_{l\neq k}J_{kl}\sigma'_l\sigma'_k-h_i\sigma'_k\delta_{k,i}\right]}}{\sum_{\sigma=\pm1}e^{-\beta\left[\sum_{l\neq k}J_{kl}\sigma'_l\sigma-h_i\sigma\delta_{k,i}\right]}}. \qquad (8)$$

The transition rates are identical to the case $h_i=0$ apart from the single-spin flip involving the spin σ_i. Using the Bayes relation and the master equation (3), the average of the spin σ_i at time t can be expanded to lowest order in Δs under the following form:

$$\begin{aligned}\langle\sigma_i(t)\rangle&=\sum_{\{\sigma\}}\sigma_i\,\wp(\{\sigma\},t)\\&=\sum_{\{\sigma\},\{\sigma'\}}\sigma_i\,\wp(\{\sigma\},t|\{\sigma'\},s+\Delta s)\wp(\{\sigma'\},s+\Delta s)\end{aligned}$$

$$= \sum_{\{\sigma\},\{\sigma'\}} \sigma_i \,\wp(\{\sigma\}, t|\{\sigma'\}, s+\Delta s)\Big[(1-\Delta s)\wp(\{\sigma'\}, s) + \Delta s \sum_{\{\sigma''\}} \wp(\{\sigma''\}, s) W_h(\{\sigma''\} \rightarrow \{\sigma'\})\Big]. \quad (9)$$

W_h being the only quantity depending on the magnetic field in equation (9), the first term disappears after a derivative with respect to the magnetic field. In the last term, the single-spin flip involving the spin σ_i, i.e. the one coupled to the magnetic field, is the only one that gives a non-vanishing contribution. The integrated response function between the time s and $s+\Delta s$ is $\left[\frac{\partial\langle\sigma_i(t)\rangle}{\partial h_i}\right]_{h_i\rightarrow 0}$ and the limit $\Delta s \rightarrow 0$ leads to the response function:

$$\lim_{\Delta s\rightarrow 0} \frac{1}{\Delta s}\left[\frac{\partial\langle\sigma_i(t)\rangle}{\partial h_i}\right]_{h_i\rightarrow 0} = \lim_{\Delta s\rightarrow 0} \frac{1}{\Delta s}\int_s^{s+\Delta s} R_{ii}(t,u)du = R_{ii}(t,s). \quad (10)$$

According to the definition of the response function (10), the calculation can be limited to the lowest order in Δs. As a consequence, the conditional probability in equation (9) can be replaced by $\wp(\{\sigma\}, t|\{\sigma'\}, s)$.

3. Equilibrium fluctuation-dissipation relation

3.1. The response function

If the system is in thermal equilibrium at time s, the probability distribution $\wp(\{\sigma\}, s)$ has to be replaced in equation (9) by $\wp_{\rm eq}(\{\sigma\})$. Then the sum over $\{\sigma''\}$ can be calculated:

$$\sum_{\{\sigma''\}} \wp_{\rm eq}(\{\sigma''\}) W_h(\{\sigma''\} \rightarrow \{\sigma'\})$$
$$= \sum_{\{\sigma''\}} \frac{1}{\mathcal{Z}} e^{-\beta\sum_{k,l<k} J_{kl}\sigma''_k\sigma''_l} \times \left[\prod_{j\neq i} \delta_{\sigma''_j,\sigma'_j}\right] \frac{e^{-\beta\left[\sum_{j\neq i} J_{ij}\sigma'_i\sigma'_j - h_i\sigma'_i\right]}}{\sum_{\sigma_i^{(3)}=\pm 1} e^{-\beta\left[\sum_{j\neq i} J_{ij}\sigma_i^{(3)}\sigma'_j - h_i\sigma_i^{(3)}\right]}}$$
$$= \wp_{\rm eq}(\{\sigma'\}) e^{\beta h_i\sigma'_i} \frac{\cosh\left(\beta\sum_{j\neq i} J_{ij}\sigma'_j\right)}{\cosh\left(\beta\left[\sum_{j\neq i} J_{ij}\sigma'_j - h_i\right]\right)}. \quad (11)$$

The derivative with respect to h_i followed by the limit $h_i \rightarrow 0$ gives $\beta\wp_{\rm eq}(\{\sigma'\})[\sigma'_i - \tanh\left(\beta\sum_{j\neq i} J_{ij}\sigma'_j\right)]$. When replaced in equation (9), one obtains the following integrated response function

$$\left[\frac{\partial\langle\sigma_i(t)\rangle}{\partial h_i}\right]_{h_i\rightarrow 0} = \beta\Delta s\left[\langle\sigma_i(t)\sigma_i(s)\rangle - \langle\sigma_i(t)\tanh\Big(\beta\sum_{j\neq i} J_{ij}\sigma_j(s)\Big)\rangle\right] \quad (12)$$

and according to equation (10) the response function reads

$$R_{ii}(t,s) = \beta\left[\langle\sigma_i(t)\sigma_i(s)\rangle - \langle\sigma_i(t)\tanh\Big(\beta\sum_{j\neq i} J_{ij}\sigma_j(s)\Big)\rangle\right]. \quad (13)$$

3.2. Equivalence with the usual expression

The equilibrium fluctuation-dissipation theorem states that the response function is related to the time-derivative of the correlation function. We will now show that the expression (13) is compatible with this statement. At equilibrium, the correlation function is invariant under a time-translation. As a consequence, one has the relation

$$\frac{\partial C_{ii}(t,s)}{\partial t} = -\frac{\partial C_{ii}(t,s)}{\partial s}. \tag{14}$$

Moreover, it can be shown that the conditional probability $\wp(\{\sigma\}, t|\{\sigma'\}, s)$ satisfies the master equation (3) for the time-variable t and a similar equation for s:

$$\left(1 - \frac{\partial}{\partial s}\right)\wp(\{\sigma\}, t|\{\sigma'\}, s) = \sum_{\{\sigma''\}} \wp(\{\sigma\}, t|\{\sigma''\}, s)W(\{\sigma'\} \to \{\sigma''\}). \tag{15}$$

The time-derivative of the correlation function is then

$$\begin{aligned}
\frac{\partial C_{ii}(t,s)}{\partial t} &= \sum_{\{\sigma\},\{\sigma'\}} \sigma_i\sigma'_i \frac{\partial\wp(\{\sigma\}, t|\{\sigma'\}, s)}{\partial t}\wp_{\rm eq}(\{\sigma'\}) \\
&= -\sum_{\{\sigma\},\{\sigma'\}} \sigma_i\sigma'_i \frac{\partial\wp(\{\sigma\}, t|\{\sigma'\}, s)}{\partial s}\wp_{\rm eq}(\{\sigma'\}) \\
&= -C_{ii}(t,s) + \sum_{\{\sigma\},\{\sigma'\},\{\sigma''\}} \sigma_i\sigma'_i\wp(\{\sigma\}, t|\{\sigma''\}, s)W(\{\sigma'\} \to \{\sigma''\})\wp_{\rm eq}(\{\sigma'\}).
\end{aligned} \tag{16}$$

The sum over $\{\sigma''\}$ can be performed on the lines of equation (11) for the Ising-Glauber model. One obtains

$$\begin{aligned}
\sum_{\{\sigma'\}} \sigma'_i W(\{\sigma'\} \to \{\sigma''\})\wp_{\rm eq}(\{\sigma'\}) &= \frac{1}{\mathcal{Z}} \sum_{\{\sigma'\}} \sigma'_i \frac{\left[\prod_{j\neq i}\delta_{\sigma'_j,\sigma''_j}\right] e^{-\beta\sum_{j\neq i} J_{ij}\sigma''_i\sigma''_j}}{\sum_{\sigma_i^{(3)}=\pm1} e^{-\beta\sum_{j\neq i} J_{ij}\sigma_i^{(3)}\sigma''_j}} e^{-\beta\sum_{k,l<k} J_{kl}\sigma'_k\sigma'_l} \\
&= \wp_{\rm eq}(\{\sigma''\}) \tanh\left(\beta\sum_{j\neq i} J_{ij}\sigma''_j\right).
\end{aligned} \tag{17}$$

Replacing in (16) and identifying with (13), one gets the expression of the equilibrium fluctuation-dissipation theorem for the Ising-Glauber model:

$$R_{ii}(t,s) = \beta\frac{\partial C_{ii}(t,s)}{\partial s} = \beta\left[\langle\sigma_i(t)\sigma_i(s)\rangle - \langle\sigma_i(t)\tanh\Big(\beta\sum_{j\neq i} J_{ij}\sigma_j(s)\Big)\rangle\right]. \tag{18}$$

4. General fluctuation-dissipation relation

Calculations have been made up to now within the hypothesis that the system is at equilibrium at time s. We will now derive a relation valid even if the system is far from equilibrium. We start with the expansion (9) of the average $\langle\sigma_i(t)\rangle$. W_h being the only quantity depending on the magnetic field, the integrated response function between the time s and $s + \Delta s$ is to lowest order in Δs

$$\left[\frac{\partial\langle\sigma_i(t)\rangle}{\partial h_i}\right]_{h_i\to0} = \Delta s \sum_{\substack{\{\sigma\},\{\sigma'\},\\ \{\sigma''\}}} \sigma_i\,\wp(\{\sigma\}, t|\{\sigma'\}, s)\left[\frac{\partial W_h}{\partial h_i}(\{\sigma''\} \to \{\sigma'\})\right]_{h_i\to0}\wp(\{\sigma''\}, s). \tag{19}$$

The derivative of the transition rate W_h defined by equation (8) is easily taken and reads

$$\left[\frac{\partial W_h}{\partial h_i}(\{\sigma''\}\to\{\sigma'\})\right]_{h_i\to 0}=\beta W(\{\sigma''\}\to\{\sigma'\})\left[\sigma_i'-\tanh\left(\beta\sum_{j\neq i}J_{ij}\sigma_j'\right)\right]. \tag{20}$$

Combining (19) and (20), the integrated response function is rewritten as

$$\begin{aligned}\left[\frac{\partial\langle\sigma_i(t)\rangle}{\partial h_i}\right]_{h_i\to 0}&=\Delta s\beta\sum_{\substack{\{\sigma\},\{\sigma'\},\\ \{\sigma''\}}}\sigma_i\sigma_i'\,\wp(\{\sigma\},t|\{\sigma'\},s)W(\{\sigma''\}\to\{\sigma'\})\wp(\{\sigma''\},s)\\ &\quad-\Delta s\beta\sum_{\substack{\{\sigma\},\{\sigma'\},\\ \{\sigma''\}}}\sigma_i\,\wp(\{\sigma\},t|\{\sigma'\},s)W(\{\sigma''\}\to\{\sigma'\})\\ &\qquad\times\tanh\left(\beta\sum_{j\neq i}J_{ij}\sigma_j'\right)\wp(\{\sigma''\},s).\end{aligned} \tag{21}$$

In the first term of (21), the sum over $\{\sigma''\}$ can be performed using the master equation (3) and the expression reorganised using the fact that after the limit $h_i\to 0$, the conditional probability becomes invariant under a time-translation and depends only on the difference $t-s$. One obtains

$$\begin{aligned}&\sum_{\substack{\{\sigma\},\{\sigma'\},\\ \{\sigma''\}}}\sigma_i\sigma_i'\,\wp(\{\sigma\},t|\{\sigma'\},s)W(\{\sigma''\}\to\{\sigma'\})\wp(\{\sigma''\},s)\\ &\quad=\sum_{\{\sigma\},\{\sigma'\}}\sigma_i\sigma_i'\,\wp(\{\sigma\},t|\{\sigma'\},s)\left(1+\frac{\partial}{\partial s}\right)\wp(\{\sigma'\},s)\\ &\quad=C_{ii}(t,s)+\frac{\partial C_{ii}(t,s)}{\partial s}-\sum_{\{\sigma\},\{\sigma'\}}\sigma_i\sigma_i'\frac{\partial\wp}{\partial s}(\{\sigma\},t|\{\sigma'\},s)\wp(\{\sigma'\},s)\\ &\quad=C_{ii}(t,s)+\frac{\partial C_{ii}(t,s)}{\partial s}+\frac{\partial C_{ii}(t,s)}{\partial t}.\end{aligned} \tag{22}$$

Similarly, in the second term of equation (21) the sum over $\{\sigma''\}$ can be performed using the master equation (3) and leads to

$$\begin{aligned}&\sum_{\substack{\{\sigma\},\{\sigma'\},\\ \{\sigma''\}}}\sigma_i\,\wp(\{\sigma\},t|\{\sigma'\},s)\tanh\left(\beta\sum_{j\neq i}J_{ij}\sigma_j'\right)W(\{\sigma''\}\to\{\sigma'\})\wp(\{\sigma''\},s)\\ &\quad=\sum_{\{\sigma\},\{\sigma'\}}\sigma_i\,\wp(\{\sigma\},t|\{\sigma'\},s)\tanh\left(\beta\sum_{j\neq i}J_{ij}\sigma_j'\right)\left(1+\frac{\partial}{\partial s}\right)\wp(\{\sigma'\},s)\\ &\quad=\left(1+\frac{\partial}{\partial s}+\frac{\partial}{\partial t}\right)\sum_{\{\sigma\},\{\sigma'\}}\sigma_i\,\wp(\{\sigma\},t|\{\sigma'\},s)\tanh\left(\beta\sum_{j\neq i}J_{ij}\sigma_j'\right)\wp(\{\sigma'\},s).\end{aligned} \tag{23}$$

Putting together equations (22) and (23) into (21), one can then evaluate the response function (10):

$$R_{ii}(t,s)=\beta\left(1+\frac{\partial}{\partial s}+\frac{\partial}{\partial t}\right)\left[C_{ii}(t,s)-\langle\sigma_i(t)\tanh\left(\beta\sum_{j\neq i}J_{ij}\sigma_j(s)\right)\rangle\right]. \tag{24}$$

The hyperbolic tangent is the equilibrium value of a single spin σ_i in the Weiss field created by all other spins at time s. Moreover, the hyperbolic tangent being an odd function of its argument and since $\sigma_i^2 = 1$, one can rewrite (24) in the following form:

$$R_{ii}(t,s) = \beta\left(1+\frac{\partial}{\partial s}+\frac{\partial}{\partial t}\right)\Big[C_{ii}(t,s) - \langle\sigma_i(t)\sigma_i(s)\tanh\Big(\beta\epsilon_i(s)\Big)\rangle\Big]. \qquad (25)$$

where $\epsilon_i(s) = \sum_{j\neq i} J_{ij}\sigma_i(s)\sigma_j(s)$ is the energy at site i.

5. Conclusion

The expression (24) (or (25)) of the response function makes apparent the way the FDT is violated. At equilibrium, all averages are invariant under a time-translation, i.e. depend only on $t-s$ so the derivatives over s and t cancel and at equilibrium the average in equation (24) is equal to the time-derivative of the correlation function as shown in section 3.2. The expression (24) is very general. Since the response function is expressed as thermodynamic averages, it does not depend on the initial conditions. Moreover, it does not depend on the dimension of space or whether or not, the lattice is regular. It applies to any configuration of exchange couplings so for a disordered system, the average response function is just the average of expression (24) over all couplings configurations. Equations (22) and (23) suggest that the presence of the term $1+\frac{\partial}{\partial s}+\frac{\partial}{\partial t}$ in the expression of the response function may be a general feature of the response function out-of-equilibrium. Exact results for other models are highly desirable. The last term of (24) whose equilibrium limit is the time-derivative of the correlation function may also be evaluated perturbatively for certain models.

This work may also help to improve numerical simulations. Up to now, the FDT has been numerically checked by calculating the time-integrated response function. One can note that equation (19) can be used to calculate the response function directly during a Monte Carlo simulation.

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